

Minimal duality breaking in the Kallen-Lehman approach to 3D Ising model: a numerical test

Marco Astorino^{1,4} *, Fabrizio Canfora¹ †,
Cristián Martínez^{1,5} ‡, Luca Parisi^{2,3} §

¹*Centro de Estudios Científicos (CECS), Valdivia, Chile*

²*Istituto Nazionale di Fisica Nucleare, GC di Salerno, Italy*

³*Dipartimento di Fisica E. R. Caianiello, Università di Salerno, Italy*

⁴*Instituto de Física, Pontificia Universidad Católica de Valparaíso, Chile*

⁵*Centro de Ingeniería de la Innovación del CECS (CIN), Valdivia, Chile*

February 20, 2009

Abstract

A Kallen-Lehman approach to 3D Ising model is analyzed numerically both at low and high temperature. It is shown that, even assuming a minimal duality breaking, one can fix three parameters of the model to get a very good agreement with the MonteCarlo results at high temperatures. With the same parameters the agreement is satisfactory both at low and near critical temperatures. How to improve the agreement with MonteCarlo results by introducing a more general duality breaking is shortly discussed.

Keyword: Regge theory, Ising model, spin glasses.

PACS: 12.40.Nn, 11.55.Jy, 05.20.-y, 05.70.Fh.

CECS-PHY-08/01

Introduction

The three dimensional Ising model (henceforth 3DI) is one of the main open problems in field theory and statistical mechanics. A large number of interesting statistical systems near the transition point are described by 3DI and the

*marco.astorino AT gmail.com

†canfora AT ceecs.cl

‡martinez AT ceecs.cl

§parisi AT sa.infn.it

theoretical methods suitable to deal with such a problem manifest deep connections in various areas of physics ranging from quantum information theory to string theory (for a review see e.g. [1]). Besides its intrinsic interest in statistical physics, since the formulation of the Svetitsky-Yaffe conjecture [2], it has been widely recognized its role in describing the deconfinement transition in QCD. For this reason, the 3D Ising model is worth to be further investigated.

It has been recently proposed [3] to use in statistical mechanics the powerful tools of Regge theory [4, 5] which have been so fruitful in the study of the strong interactions leading to the formulation of the dual models [6] (two detailed reviews are [7] and [8]). It has been argued in [9] that such ideas may be useful in dealing with the 3D Ising model. It would be also interesting to try to test these methods in the mean field theory of spin glass¹ as developed in [13] (recently it has been proved, that such a framework provides one with the exact solution in the mean field Ising spin glass [14, 15, 16]).

In the present paper we perform a numerical test of these methods in the case of the 3D Ising model. We will try to find the best "Regge parameters" appearing in the Kallen-Lehman form for the free energy: that is the parameters which provide one with the best possible agreement both at high and low temperatures MonteCarlo expansions as well as around the critical point.

The paper is organized as follows: in the second section the Kallen-Lehman form for the free energy of the 3D Ising model is discussed. In the third section the issue of duality breaking is analyzed. In the fourth and fifth sections the comparison with MonteCarlo results at high and low temperatures are presented. In the sixth section, the behavior at the critical point is described. In the seventh section some possible improvements are pointed out. Eventually, we draw some conclusions.

¹Detailed reviews on the subject are [10] [11] [12].

1 The Kallen-Lehman form for the free energy

The Kallen-Lehman representation [9] gives rise to an ansatz for the free energy of the 3DI model of the following form²

$$F_{3D}^{(\zeta_i, \lambda)}(\beta) = F_{2D}(\beta) + \frac{\lambda}{(2\pi)^2} \int_0^\pi dz \int_0^\pi dy \cdot \log \left\{ \frac{1}{2} \left[1 + \left(1 - \left[2 \frac{(\Delta(z) - 1)^{\zeta_1}}{\Delta(z)} \right]^{\zeta_2} \sin^2 y \right)^{\zeta_3} \right] \right\}, \quad (1)$$

$$F_{2D}(\beta) = F_{1D}(\beta) + \frac{1}{2\pi} \int_0^\pi dx \log \left\{ \frac{1}{2} \left[1 + \sqrt{1 - k_{eff}(\beta)^2 \sin^2 x} \right] \right\}, \quad (2)$$

$$F_{1D}(\beta) = \log 2 \cosh q\beta, \quad \Delta(z) = \left(1 + (1 - k_{eff}(\beta)^2 \sin^2 z)^{\zeta_0} \right)^2, \quad (3)$$

$\zeta_1, \zeta_2, \zeta_3 > 0, \quad q = 2$

here, for sake of simplicity, we consider $\zeta_1 = 1/2 = \zeta_3$ (the 2D Ising values). In order to avoid a complex free energy (which could arise due to the two square roots),

$$0 \leq k_{eff}(\beta) \leq 1 \Rightarrow \quad (4)$$

$$1 \leq \Delta(z) \leq 4 \quad \vee \quad \zeta_2 > 0 \Rightarrow$$

$$0 \leq \left[2 \frac{(\Delta(z) - 1)^{1/2}}{\Delta(z)} \right]^{\zeta_2} \leq 1, \quad (5)$$

$$u = \exp(-2\beta), \quad t = \tanh \beta. \quad (6)$$

At high temperatures it is convenient the variable $t = \tanh \beta$ while $u = \exp(-2\beta)$ is the standard variable at small temperatures. Thus our trial free energy will depend on 3 parameters $\lambda, \zeta_2 := \nu, \zeta_0 := \zeta$ to be fixed in comparison with MonteCarlo data.

The natural value (suggested by the application of Regge theory) of the factor q in the trivial one dimensional term in Eq. (3) is $q = 2$ (and this is the value that we will consider from now on, see [9]) since the one dimensional term of exact solution of the 2D Ising model is precisely $\log 2 \cosh 2\beta$. On the other hand, we have also obtained quite good numerical results for $q = 1$: in particular, for the set of parameters

$$\zeta_{q=1}^* = 1.096, \quad \nu_{q=1}^* = 2.586, \quad \lambda_{q=1}^* = 0.127 \quad (7)$$

²The "Regge parameters" appearing in these formulas are related with those appearing in [9] by the following identities $\zeta_1 = \nu, \zeta_3 = 1/2 = \zeta_2, \zeta_0 = \alpha$.

we get the following deviations at high and small temperatures

$$\sigma_{HT}(\zeta_{q=1}^*, \nu_{q=1}^*, \lambda_{q=1}^*) \approx \sqrt{\frac{\chi(\zeta_{q=1}^*, \nu_{q=1}^*, \lambda_{q=1}^*)}{50}} \approx 10^{-6} \quad (8)$$

$$\sigma_{LT}(\zeta_{q=1}^*, \nu_{q=1}^*, \lambda_{q=1}^*) \approx \frac{\sqrt{\chi_{LT}(\zeta_{q=1}^*, \nu_{q=1}^*, \lambda_{q=1}^*)}}{\sqrt{50}} \approx 10^{-3} \quad (9)$$

(a definition of σ_{HT} and σ_{LT} will be provided in the next sections in Eqs. (20), (22), (25) and (26)). These quite small deviations obtained with $q = 1$ (which indeed is less natural than the ansatz with $q = 2$) show that the present method is well suited to describe the thermodynamics of the 3D Ising model. In any case, as it will be shown in a moment, the results for $q = 2$ are quite better.

Besides the first trivial term in Eq. (3), the "Regge free energy" depends on the temperature through an effective $k_{eff}(\beta)$ in the same way as the (non trivial part of the) free energy of the 2D Ising model depends on β :

$$(k_{2D}(\beta))^2 = \left(\frac{2}{\cosh 2\beta \coth 2\beta} \right)^2 = \left(4 \frac{\exp(2\beta) - \exp(-2\beta)}{(\exp(2\beta) + \exp(-2\beta))^2} \right)^2. \quad (10)$$

The duality symmetry of the 2D Ising model (discovered in [17] by Kramers and Wannier before the exact solution of Onsager [18]) is manifest in the above function of the temperature since $k(\beta)$ has the same expression when rephrased in terms of the low temperatures variable u and the high temperatures variable t . Indeed, the 3D Ising model has not such a duality symmetry: in the next section it will be described how the simplest duality breaking can be achieved.

2 Minimal duality breaking

There are indeed many reasonable ways to break duality, how can one choose? Here a criterion of simplicity will be followed. An important ingredient is the following: all the Ising models on simple hypercubic lattices are invariant under the Marčesini-Shrock transformation [19]

$$\beta \rightarrow \beta + in \frac{\pi}{2}, \quad n \in \mathbb{Z}.$$

While this symmetry is obviously realized in the 2D case in which one has at own disposal the exact solution, such an exact symmetry puts a strong constraint on the form of the free energy. As discussed in [9], the free energy suggested by the Kallen-Lehman representation is expect to depend on (a suitable) $k_{eff}(\beta)$. A simplicity criterion (which, as it will be shown in a moment, is supported by the numerical data) suggests to consider the easiest possible modification of the k of the 2D case in Eq. (10):

$$k_{eff}(\beta) = \frac{4}{d_1} \frac{d_3 \exp(2\beta) - d_2 \exp(-2\beta)}{(\exp(2\beta) + d_0 \exp(-2\beta))^2}, \quad (11)$$

the fact that the exponential only depend on 2β is the simplest possible way to fulfil the Marchesini-Shrock symmetry. The four parameters d_i ($i = 0, \dots, 3$) are not independent since there are two conditions that the function k_{eff} has to fulfil: firstly, the maximum of k_{eff} has to occur at the known critical temperature $(\beta^*)^{-1}$ of the 3D Ising model:

$$\beta^* | \partial_\beta k_{eff}(\beta) |_{\beta=\beta^*} = 0 \quad (12)$$

$$\beta^* = 0.22165. \quad (13)$$

The second condition is related to the fact that the expected transition has to occur [9] when $k_{eff}(\beta) = 1$ as it happens in the 2D case:

$$k_{eff}(\beta^*) = 1. \quad (14)$$

Thus, in order to consider the simplest modification of the two-dimensional $k(\beta)$ in Eq. (10), we will take $d_3 = 1$ (the 2D Ising value) in such a way that only one parameter is left: d_1 and d_2 can be expressed in terms of d_0 and β^* as follows

$$d_2 = \frac{\exp(4\beta^*) - 3d_0}{3 - d_0 \exp(-4\beta^*)}; \quad (15)$$

$$d_1 = 4 \left[\frac{\exp(2\beta^*) - \left(\frac{\exp(4\beta^*) - 3d_0}{3 - d_0 \exp(-4\beta^*)} \right) \exp(-2\beta^*)}{(\exp(2\beta^*) + d_0 \exp(-2\beta^*))^2} \right]. \quad (16)$$

From the numerical point of view, this parametrization is very useful since automatically ensures that the maximum is equal to one avoiding possible problems related to negative numbers appearing inside the square root in Eq. (2). Moreover the minimal modification criterion suggests that

$$d_0 = 1 \quad (17)$$

as in the 2D case.

Indeed, one should expect a more general duality breaking: the 2D Ising model and its exact duality are closely related to $\mathbf{N}=4$ SUSY Yang-Mills theory (for instance see [20]). From the gauge theory side, one would thus expect that a minimal duality breaking should be related to a Yang-Mills theory with two supersymmetry which has an effective duality (for instance see [21]). The 3D Ising model is related to QCD without supersymmetries, so that it is natural to expect that a more general pattern of duality breaking (which will be discussed later on) should occur in the 3D Ising model. However, it is a truly remarkable feature of the present tools that already a minimal duality breaking works very well in comparisons with MonteCarlo results. It is worth to mention here that the so called "effective string approach" to the 3D Ising model (in which duality symmetry is unbroken) gives reasonable results in comparison with MonteCarlo data (see for instance [22]).

One can express k_{eff} in terms of the high and low temperatures variables:

$$k_{eff}(u) = \frac{4}{d_1} \frac{u(1 - d_2 u^2)}{(1 + d_0 u^2)^2}, \quad (18)$$

$$k_{eff}(t) = \frac{4(1 - t^2)}{d_1} \frac{[t^2(1 - d_2) - 2t(1 + d_2) + (1 - d_2)]}{[t^2(1 + d_0) - 2t(1 - d_0) + (1 + d_0)]^2}. \quad (19)$$

so our ansatz for the 3D Ising free energy is given by Eq. (1) in which k_{eff} is in Eq. (11) with the constants in Eqs. (15), (16) and (17).

3 High temperatures

The idea is to find the best set of high temperatures parameters ($\zeta_0^*, \zeta_2^*, \lambda^*$) in Eqs. (1), (3) (with the constraints in Eqs. (15), (16) and (17)) which reproduces as close as possible the available Monte Carlo data (see [23]). A hypercubic lattice has been chosen in the parameters space (every point in the lattice representing a possible set of high temperature parameters), then the free energy (1) will be evaluated at every point in the lattice. The best choice of parameters will be the one minimizing the following deviation function which, to some extent, represents the deviation between the ansatz and the Monte Carlo data:

$$\chi(\zeta, \nu, \lambda) = \sum_i^{50} \left| F_{3D}^{(\zeta, \nu, \lambda)}(\beta_i) + I_0 - F_{HT}^{MC}(\beta_i) \right|^2, \quad (20)$$

$$\beta_i - \beta_{i-1} = \frac{0.03}{50}, \quad \beta_{50} = \beta_{max} = 0.03, \quad I_0 = 2.4831$$

$$F_{HT}^{MC}(\beta) = 3 \cosh \beta + \left(3 (\tanh \beta)^4 + 22 (\tanh \beta)^6 + 187.5 (\tanh \beta)^8 + 1980 (\tanh \beta)^{10} + 24044 (\tanh \beta)^{12} + 319170 (\tanh \beta)^{14} + \dots \right)$$

where we keep the terms up to the 15th of [23] since our algorithm is not sensitive to the higher order terms, F_{HT}^{MC} is the high temperatures MonteCarlo free energy, β_m can be assumed to be of order 0.03³ and I_0 is a constant introduced for numerical convenience⁴.

In order to compare the Regge coefficients with the high temperature coefficients in [23], we need to change variable from β to $t = \tanh \beta$, so that we have to use the expression in Eq. (19) whenever it appears k_{eff} .

³After $\beta \approx 0.05$ one is not anymore in the high temperatures regime since the critical temperature is at $\beta^* \approx 0.22$ which is only a factor of four larger. Indeed, $\beta \approx 0.03$ appears to be not enough smaller than β^* . Nevertheless, we will see that the agreement of the Regge free energy with MonteCarlo data is excellent up to $\beta \approx 0.03$.

⁴In order for the program to be able to select good points in the parameters space an arbitrary constant has to be added. Otherwise, the C++ program would select uncorrect functions: for instance, it would select two curves which intersect in a point near $\beta = 0$ (but whose shapes are very different) instead of two parallel curves.

The set of points candidates to be the best parameters are:

$$\zeta^* = 1.9389, \quad \nu^* = 1.9205, \quad \frac{\lambda^*}{(2\pi)^2} = 0.0781 \quad (21)$$

In order to have a graphical idea of the closeness of the Regge and the MonteCarlo free energies at high temperature we have drawn in Fig. (1) both functions. The agreement appears to be excellent: the deviation at high temperature is

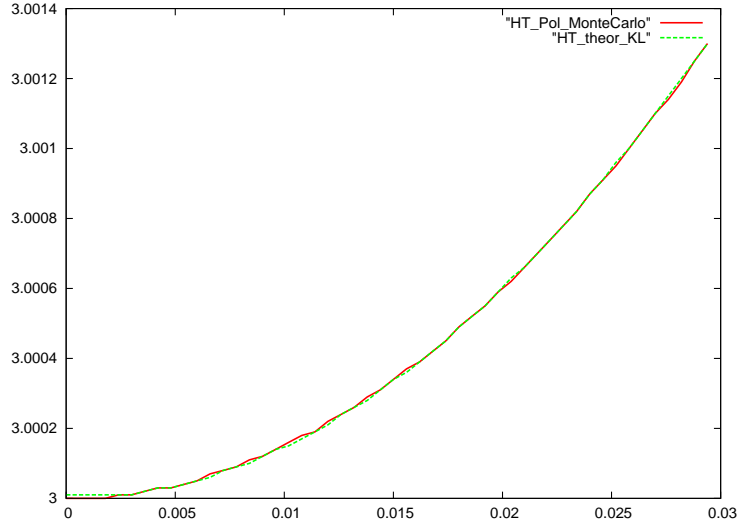
$$\sigma_{HT}(\zeta^*, \nu^*, \lambda^*) \approx \sqrt{\frac{\chi(\zeta^*, \nu^*, \lambda^*)}{50}} \approx 10^{-6}. \quad (22)$$

It is worth to note that in the range of parameters

$$1 \leq \zeta^* \leq 2, \quad 1.5 \leq \nu^* \leq 2.5, \quad 0.05 \leq \lambda^* \leq 0.2$$

we found many other good sets of parameters with only slightly larger deviations with respect to the MonteCarlo free energy. However, as it will be discussed in a moment, it is very difficult to evaluate the errors on the single coefficients of the expansions. Thus, we simply considered the set in Eq. (21) but other sets of parameters in the above range could reproduce better the single coefficients.

Figure 1: MonteCarlo $F_{HT}^{MC}(\beta)$ and Kallen-Lehman $F_{3D}^{(\zeta^*, \nu^*, \lambda^*)}(\beta)$ free energies at high temperatures versus β .



There are some points in the parameters space in which the agreement at low temperatures is much better than the agreement at high temperatures (which is

in any case quite good). In the present analysis it is apparent that one cannot achieve an excellent agreement both at high and at low temperatures: in the best cases very small deviations (of the order of 10^{-6}) on one side correspond on the other side to quite good but not excellent deviation of the order of 10^{-4} . This is a manifestation of the already discussed fact that the 3D Ising model, being related to QCD without any supersymmetry, needs a more general duality breaking.

3.1 Numerical Derivatives at high temperatures

A consistency test would be provided comparing the derivatives of MonteCarlo free energy with the ones predicted by our model at $\beta = 0$. Due to the complicated expression of the Regge free energy numerical methods are needed. To this aim we consider the finite difference approximation of the derivative which, at any order of derivation n , is given by the forward finite difference of order n divided by the increase of the independent variable (say δ) raised to the n -th power, i.e.

$$\frac{d^n F_{3D}^{(\zeta^*, \nu^*, \lambda^*)}}{d\beta^n}(\beta) = \frac{\Delta_\delta^n [F_{3D}^{(\zeta^*, \nu^*, \lambda^*)}](\beta)}{\delta^n} + O(\delta)$$

$\Delta_\delta^n[f](x)$ being the n -th order finite difference. Behind this apparently easy procedure there are hidden dangers which already at the lowest orders deserve special attention (for an introductory discussion see [24]): which is the best choice of δ in order to approximate correctly the value of the n -th order derivative (since neither too small nor too large values are correct)? One can only try to find the suitable $\delta_{(n)}$ to reproduce the MonteCarlo coefficients at any order. In the case of the Regge free energy it's always possible to find (more than) one suitable numerical value for δ . One can verify that the $\delta_{(n)}$ which reproduce the MonteCarlo results fulfil a sort of "natural" scaling (see [24]): namely, as the order of derivation increases, the suitable δ reproducing the MonteCarlo result stays constant or decreases. Despite being only a first attempt to compute the derivatives of the Regge partition function in zero, nevertheless it is a quite encouraging fact that at any order one can find at least one δ reproducing exactly the MonteCarlo data.

Another possible way to obtain the numerical derivatives for $\beta = 0$ is the following. One can fit the Regge free energy (in which now the parameters are fixed to be the best parameters) for small β with a polynomial with unknown coefficients (in which *a priori* one has to include all the even and odd-coefficients) in such a way that the coefficients of the polynomial are the numerical derivatives at the origin. However, after the first four coefficients are fixed, the polynomial becomes very close to the Regge free energy. The higher order coefficients are fixed by the program to be the MonteCarlo results, but it is very difficult to evaluate the errors since if one changes the higher order coefficients of a factor of two or four the deviation with respect to the optimal polynomial is smaller than 10^{-6} . Even with this method, it is extremely difficult to evaluate the deviations of the derivatives of the higher order derivatives of the Regge free energy from

the MonteCarlo results. In any case, we find an attractive feature of our model that even fixing the first few coefficients at high temperature one obtains a good agreement at the critical point and at low temperatures.

4 Low temperatures

Once the best set of high temperatures parameters $(\zeta^*, \nu^*, \lambda^*)$ have been found in Eq. (21) one could hope to find a good agreement also at low temperatures (something which, *a priori*, is very far from obvious). The internal energy at low temperatures is (k_{eff}) as in Eq. (18) and expressing F_{1D} as in (3) in terms of u)

$$\left\langle \frac{E}{N} \right\rangle^{KL}(u) + 2I_1 = 2u \frac{\partial}{\partial u} F_{3D}^{(\zeta, \nu, \lambda)}(u). \quad (23)$$

This is the average energy for spin (the two expressions can differ by a non zero constant I_1 , see footnote 4) to be compared with $\left\langle \frac{E}{N} \right\rangle^{MC}$ (the polynomial in u representing the MonteCarlo average energy for spin for small u) found in [25].

It is worth to discuss the origin of the constant I_1 in the above formula. The partition function of the 3D Ising model reads

$$\begin{aligned} Z_{3D} &= \sum_{\{\sigma_i\}} \exp(-\beta(H_0)), \\ H_0 &= \sum_{\langle ij \rangle} \sigma_i \sigma_j + const \end{aligned}$$

where the constant in the Hamiltonian can always be chosen in such a way that the lowest energy state has zero energy. The ansatz (1) has not been deduced by solving in some approximated way the model. Rather, it has been found on the basis of the Regge theory and the Kallen-Lehman representation: one cannot pretend that it already corresponds to the normalization in which the Hamiltonian H_0 has a zero energy ground state. At very low temperatures, the free energies corresponding to H_0 and to $H_0 + const$ differ by a term proportional to $1/T$

$$\log \left[\sum_{\{\sigma_i\}} \exp(-\beta(H_0 + const)) \right] - \log \left[\sum_{\{\sigma_i\}} \exp(-\beta(H_0)) \right] \sim \beta \sim 1/T \sim \log u.$$

In terms of the internal energy, such a term corresponds to a constant:

$$2u \frac{\partial}{\partial u} \log u = const.$$

From the numerical point of view it is extremely inconvenient to use the expression on the right hand side of Eq. (23) since the derivative ∂_u has a really big expression. A trivial but useful trick is the following: in [25] one has a

polynomial expression for the average energy for spin so that one can integrate it and obtain the Monte Carlo expression for the free energy at low temperatures:

$$\left\langle \frac{E}{N} \right\rangle^{KL}(u) + 2I_1 = 2u \frac{\partial}{\partial u} F_{LT}^{MC}(u) = \sum_{i=6}^{14} a_i^{(L)} u^i,$$

this implies that

$$F_{LT}^{MC}(u) = \frac{1}{2} \left(\sum_{i=6}^{14} \left(\frac{a_i^{(L)}}{i} \right) u^i - 2I_1 \log u \right). \quad (24)$$

Therefore, the low temperatures test function reads

$$\chi_{LT}(\zeta^*, \nu^*, \lambda^*) = \sum_{i=1}^{50} \left| F_{3D}^{(\zeta^*, \nu^*, \lambda^*)}(u_i) + I_2 - F_{LT}^{MC}(u_i) \right|^2, \quad (25)$$

$$u_i - u_{i-1} = \frac{0.3}{50}, \quad u_1 = u_{min}, \quad u_{50} = u_{max} = 0.3,$$

$$F_{LT}^{MC}(u) = \left[\frac{1}{2} \left(\frac{12}{6} (u)^6 + \frac{60}{10} (u)^{10} + \right. \right. \\ \left. \left. - \frac{84}{12} (u)^{12} + \frac{420}{14} (u)^{14} \dots \right) + I_1 \log u \right]$$

where $I_1 = -1$ and $I_2 = 0.1034$. We keep the terms up to the 15th of [25] since our algorithm is not sensitive to the higher order terms and u_{max} can be assumed to be of order 0.3.

Actually, the value of u which corresponds to the critical temperature is $u_{crit} = \exp(-2\beta_{crit}) \approx 0.6$. The low temperatures expansion provides one with reasonable results for $u \ll 0.6$. Indeed, $u_{max} \approx 0.3$ is not at all much smaller than u_{crit} : one may expect a reasonable value of u_{max} to be quite smaller than⁵ 0.01. Nevertheless, we will see that the agreement is quite good up to $u \approx 0.3$.

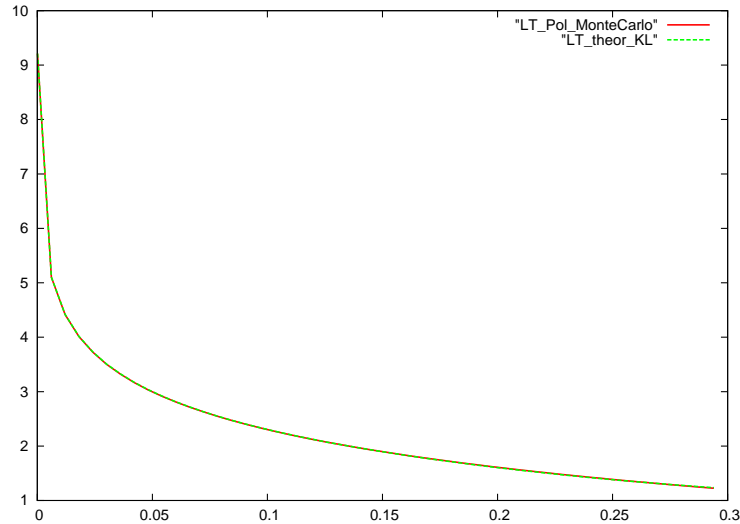
Eventually, the deviation at low temperatures between the Regge and the MonteCarlo free energies *evaluated for the same optimal parameters* in Eq. (21), which have been found by asking the optimal agreement at high temperatures is

$$\sigma_{LT}(\zeta^*, \nu^*, \lambda^*) \approx \frac{\sqrt{\chi_{LT}(\zeta^*, \nu^*, \lambda^*)}}{\sqrt{50}} \approx 10^{-5}. \quad (26)$$

and one can see that the agreement at low temperatures is two order of magnitude better than in the case in which in Eq. (3) $q = 1$ (see Eq. (9)).

⁵Unfortunately, a numerical analysis in the region of $u < 0.01$ is quite difficult because of the fact that the logarithm is very large and dominates the too small numbers coming from the MonteCarlo polynomial. If the logarithmic divergent terms would be absent, in the region $0 \leq u < 0.01$ very soon the MonteCarlo polynomial would give rise to very small numbers (below the precision of our PC). Thus, to analyze this range more refined numerical techniques are needed. In any case, the good agreement at the critical point provides one with some control on the deviation of the theoretical low temperatures coefficients with respect to the MonteCarlo ones.

Figure 2: MonteCarlo F_{LT}^{MC} and Kallen-Lehman $F_{3D}^{(\zeta^*, \nu^*, \lambda^*)}(u)$ free energies at low temperatures versus u .



Remarkably enough, at low temperatures also the agreement is quite good as can be also seen in Fig. (2). As far as the numerical derivatives at $u = 0$ of Regge free energy, the same considerations as in the high temperatures case hold. Namely, both a direct evaluation by means of a simple algorithm and to try to find the suitable approximating polynomial give results compatible with the MonteCarlo ones but it is not clear to the present authors how to estimate the errors on the single coefficients. It is nevertheless worth to stress here that the relative deviations both at high and at low temperatures are very small (see Eqs. (22) and (26)). Furthermore, as it will be now shown, also the critical exponent is in a very good agreement with the available data: one may hope that the good agreement at the critical point could prevent too large deviations of the the Kallen-Lehman derivatives from the MonteCarlo data.

5 The Critical Point

The last test is the critical point. Namely, once the parameters have been fixed as in Eq. (21) one may hope to verify that the critical point is correctly predicted too. To do this one can fit near the critical point the non-analytic part of the free energy in Eq. (1)⁶ with the optimal parameters with a function of the form

⁶That is, one has to exclude the term $\log 2 \cosh \beta$ which does not contribute to the critical behavior.

F_{CRIT}

$$F_{CRIT} \approx c_1 |\beta - \beta^*|^{2-\alpha} + c_2 \quad (27)$$

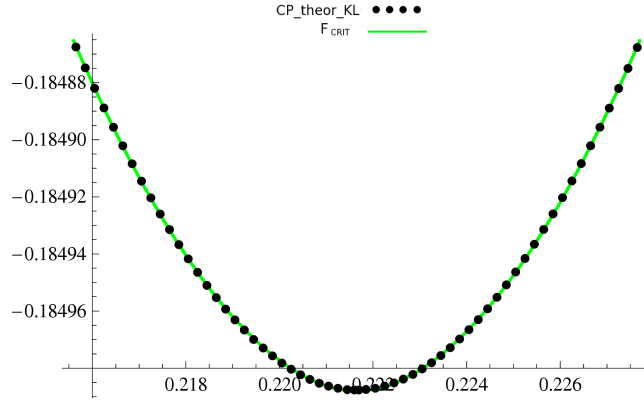
(where c_1 , c_2 and α are constant) and find the optimal values for c_1 , c_2 and α so that α will be our estimate for the critical exponent. This form of the free energy's critical part is expected both from Conformal Field Theory and experiments. The results of the fit done with the PC program *Mathematica* by fitting the (non-analytic part of the) Regge free energy with the optimal parameters in Eq. (21) with the above function (27) from $\beta_{left} = \beta^* - \Delta\beta$ to $\beta_{right} = \beta^* + \Delta\beta$ are ⁷

$$1.797 \leq c_1 \leq 1.968, \quad c_2 = -0.185, \quad 0.106 \leq \alpha \leq 0.122 \quad (28)$$

the agreement appears to be very good when compared with the recent estimate in [26] in which the authors found $\alpha_{obs} \approx 0.114(6)$ so that

$$\Delta\alpha \approx \frac{|\alpha_{obs} - \alpha|}{\alpha_{obs}} \approx \frac{7}{100} \quad (29)$$

Figure 3: Bold points represent a sampling of Kallen-Lehman free energy $F_{3D}^{(\zeta^*, \nu^*, \lambda^*)}(\beta)$ while the continuous line corresponds to the critical part of the expected free energy F_{CRIT} versus β .



Further theoretical as well as experimental determinations of α can be found in [1]: the deviation $\Delta\alpha$ of our prediction (28) from observations appears to be less than 7% in all the more recent values. The following figure Fig.(3) in which we draw both the graph of the (non-analytic part of the) Regge free energy and of F_{CRIT} confirm that in the parts of the graph of F_{CRIT} in which the dependence on α is important the agreement is satisfactory.

⁷The fit result around the critical point is stable when $0.005 \leq \Delta\beta \leq 0.006$. In this range the agreement doesn't get worse than in eq. (29) .

6 Further possible improvements

The first obvious improvement is to keep all the Regge exponents ζ_3 , ζ_2 , ζ_1 , and ζ_0 without fixing *a priori* any of them (while here, for the sake of simplicity, we set both ζ_3 and ζ_1 to 1/2, the 2D Ising values). As it has been already stressed, it is also natural to explore different patterns of duality breakings. One can keep in the parameters space the parameter d_0 without fixing it to 1 (the 2D Ising value). In the ansatz (1) the terms corresponding to the 2D Ising model (2) (which, in the Kallen-Lehman view comes from the single particles discrete part of the spectrum [9]) has a natural interpretation as a "boundary terms". In other words, the 2D-like term with a single integral has its origin in the boundary contributions in the same way as in the 2D case, the trivial one-dimensional term has its origin in the boundary. It is conceivable that the patterns of duality breakings in the bulk and at the boundary could be different. This would lead to a Kallen-Lehman free energy in which the function $k_{eff}(\beta)$ (see Eqs. (11), (15) and (16)) appearing in the purely three dimensional term (the double integral) has a d_0 different from the $k_{eff}(\beta)$ appearing in the two dimensional term (the single integral in Eq. (2)). Two different k_{eff} in the single and in the double integrals (each one with its own d_0) could describe a situation in which the pattern of duality breakings in the bulk and in the boundary are different⁸. We expect that more general duality breakings could improve of two or three order of magnitude the (already quite good) agreement at low temperatures. As a matter of fact, all these natural ways to improve the numerical results (which add at least two parameters to the computations) would need a big cluster of CPUs since without a cluster the CPU's time needed would be too long.

7 Conclusions and perspectives

In this paper a Kallen-Lehman approach to 3D Ising model has been investigated numerically in the realm of a minimal duality breaking. It has been shown that one can fix three parameters of the model to get an excellent agreement at high temperatures. *With the same set of parameters*, the agreement at low temperatures appears to be very good. Remarkably enough, *with the same set of parameters*, the predicted critical exponent α has a relative deviation with respect to the most recent determinations of the order of the 7%. We believe that the present results provide one with a strong evidence that the application of the present methods to the study of the 3D Ising model is very promising. To the best of our knowledge, there are no other analytical methods able to give reliable informations at the same time at high temperatures, at low temperatures and at the critical point. More general patterns of duality breakings are worth to be investigated since they would further improve the already very satisfactory agreement with MonteCarlo data.

⁸Also worth to be investigated is the case in which d_0 has a smooth dependence on the temperature in order to describe a pattern of duality breaking which changes with β .

Acknowledgements

This work was supported by Fondecyt grant 3070055, 1071125, 1061291, 1051056, 1051064. The Centro de Estudios Científicos (CECS) is funded by the Chilean Government through the Millennium Science Initiative and the Centers of Excellence Base Financing Program of Conicyt. F.C. kindly acknowledges Agenzia Spaziale Italiana for partial support. CECS is also supported by a group of private companies which at present includes Antofagasta Minerals, Arauco, Empresas CMPC, Indura, Naviera Ultragás and Telefónica del Sur. CIN is funded by Conicyt and the Gobierno Regional de Los Ríos. L. P. thanks PRIN SINTESI 2007 for financial support.

References

- [1] A. Pelissetto, E. Vicari, *Phys.Rept.* **368** (2002) 549.
- [2] B. Svetitsky, L. G. Yaffe, *Nucl. Phys.* **B 210**, 423 (1982).
- [3] F. Canfora, L. Parisi, G. Vilasi, *Phys.Lett.* **B638** (2006) 85.
- [4] T. Regge, *Nuovo Cimento* **14**, 951 (1959).
- [5] T. Regge, *Nuovo Cimento* **18**, 947 (1960).
- [6] G. Veneziano, *Nuovo Cimento* **57 A**, 190 (1968).
- [7] P. D. B. Collins, *Physics Report C* **1**, 103 (1971).
- [8] G. Veneziano, *Physics Report C* **9**, 199 (1974).
- [9] F. Canfora, *Phys.Lett.* **B646** (2007) 54.
- [10] M. Mezard, G. Parisi, M. Virasoro " *Spin Glass Theory and Beyond* " World Scientific, Singapore (1987).
- [11] H. Nishimori " *Statistical Physics of Spin Glasses and Information Processing: an introduction* " Oxford University Press (2001).
- [12] T. Castellani, A. Cavagna, *J. Stat. Mech.* (2005) P05012 and references therein.
- [13] G. Parisi, *Phys. Rev. Lett.* **43**, 1754 (1979); *Phys. Lett.* **73A**, 203 (1979); *J. Phys. A* **13**, L115 (1980); *J. Phys. A* **13**, 1101 (1980); *J. Phys. A* **13**, 1887 (1980); *Phys. Rev. Lett.* **50**, 1946 (1983).
- [14] F. Guerra, *Comm. Math. Phys.* **233**, 1 (2003).
- [15] F. Guerra, F. L. Toninelli, *J. Math. Phys.* **43**, 6224 (2002); *Comm. Math. Phys.* **230** (2002), 71.

- [16] M. Talagrand, *C. R. Acad. Sci. Paris, Series I* **337**, (2003) 111; *Annals of Math.* **163**, 221 (2006).
- [17] H. Kramers and G. Wannier, *Phys.Rev.* **60** (1941) 252.
- [18] L. Onsager, *Phys. Rev.* **65** (1944), 117.
- [19] G. Marchesini, R. Shrock, *Nucl. Phys.* **B 318**, 541 (1989).
- [20] C. Gomez, J. Gunnesson, R. Hernandez, " *The Ising model and planar $N=4$ Yang-Mills*" arXiv:0711.3404.
- [21] D. I. Olive, P. C. West editors, *Duality and Supersymmetric Theories*, (Cambridge University Press, 1999).
- [22] M. Caselle, M. Hasenbusch and M. Panero, JHEP **0301** (2003) 057; M. Billo, M. Caselle, L. Ferro, M. Hasenbusch and M. Panero, arXiv:0710.1751 [hep-lat].
- [23] H. Arisue, T. Fujiwara, *Phys. Rev.* **E 67**, 066109 (2003).
- [24] W. H. Press et al., " *Numerical Recipes 3rd Edition: The Art of Scientific Computing*" Cambridge University Press (2007).
- [25] G. Bhanot, M. Creutz, J. Lacki, *Phys. Rev. Lett.* **69**, 1841 (1992).
- [26] P. Butera, M. Comi, *Phys. Rev.* **B 65** (2002) 144431.